<Division of Multidisciplinary Chemistry> Molecular Aggregation Analysis

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- Molecular Aggregation Analysis -

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Scope of Research

The research at this subdivision is devoted to correlation studies on structures and properties of both natural and artificial molecular aggregates from two main standpoints: photoelectric and dielectric properties. The electronic structure of organic thin films is studied using photoemission and inverse photoemission spectrosocpies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with heterogeneous sturcutres in mocrocapsules, boipolymers, biological membranes and biological cells, and the nonlinearity in their dielectric properties is also studied in relation to molecular motions.

Research Activities (Year 2004)

Presentations

Dielectric Properties of Membranes, Asami K, 26th Annual Meeting of the Membrane Society of Japan (Tokyo, Japan), 20 - 21 May.

A Study on Thin Films of Carrier-Doped Strontium Titanate with Taking Notice of Their Interfaces with Organic Thin Films, Sato N, Harada Y, Terashima T, Kanda R, Takano M, The 12th International Conference on Solid Films and Surfaces (Hamamatsu, Japan), 21 - 25 June.

Direct Observation of Electronic Structure of Unoccupied States in Metal Phthalocyanine Thin Films, Sato N, Yoshida H, Tsutsumi K, Third International Conference on Porphyrins and Phthalocyanines (New Orleans, USA), 11 - 16 July.

Dielectric Behavior of a Microemulsion System Containing Water, Toluene and Triton X-100: Temperature dependent phase inversion, Asami K, 3rd International Conference on Broadband Dielectric Spectroscopy and its Applications, (Delft, The Netherlands), 23 - 26 August.

Electronic Structure of 2,5-Diarylsilole Derivative Thin Films Studied with Ultraviolet Photoemission and Inverse Photoemission Spectroscopies, Sato N, Yamagami T, Yoshida H, Yamaguchi S (Nagoya U.), Tamao K, Uchida M (Chisso Co.), The 8th Japan-China Joint Symposium on Conduction and Photo-conduction in Organic Solids and Related Phenomena (Okazaki, Japan), 11 - 14 November.

Dielectric Relaxation of a Nonionic Microemulsion during the Temperature-dependent Phase Inversion, Asami K, Membrane Symposium '04 (Kyoto, Japan), 18 - 19 November.

Grants

Sato N, Development of Novel Electronic Systems Based on Hybridization of Characteristic Molecular Properties and Specific Aggregate Structures, Grant-in-Aid for Scientific Research (2) on Priority Areas of Molecular Conductors, 17 October 2003 - 31 March 2008.

Yoshida H, Controlling Reactivity and Diffusion at Metal-Organic Semiconductor Interfaces through the Deposition of Metal Clusters, Grant-in-Aid for Scientific Research for Young Scientists (B), 19 October 2004 - 31 March 2006.

Study of Thin Films of Carrier-doped Strontium Titanate with Emphasis on Their Interfaces with Organic Thin Films

Carrier-doped strontium titanate (M:STO, M = V, La) thin films prepared epitaxially on single crystalline strontium titanate (STO) substrates with the pulsed laser deposition method turned out to have surface flatness, surface electric conductivities and work functions no less useful for optically transparent anode materials of organic optoelectronic devices, e.g., organic light emitting diodes in the typical architecture, than indium tin oxides (ITOs). Whereas their optical transmittance is not high enough to employ for such use at this moment, further developments on this aspect are to be expected. Among the studied STO thin films V:STO is noted for its distinguished properties. The physical properties of M:STOs appear to depend on the site of atomic substitution involving charge carrier doping in their perovskite structures, which suggests that further optimization of dopant atoms and doping levels will lead to a transparent anode material with much higher performance. The observed difference in interfacial behaviors of energy levels of cupper phthalocyanine (CuPc) overlayers between V:STO and ITOs using ultraviolet photoemission spectroscopy, that is, monotonous energy decreases of both the hole conduction level and the vacuum level with increasing thickness observed for an CuPc overlayer only on V:STO (see Figure 1), seems to demonstrate the effect by higher surface flatness of the V:STO substrate. On the very flat surface the molecular orientational change depending on the layer thickness will be expected and such a behavior may cause the monotonous change of the energy levels mentioned above. Finally, this work was carried out in collaboration with Professor Takano's group.

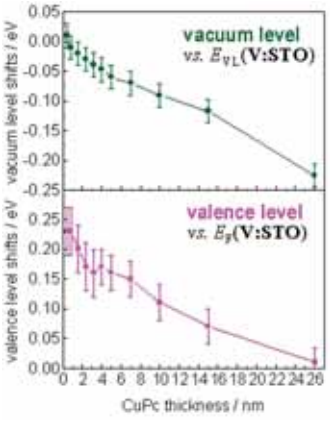

Figure 1. Thickness dependence of the apparent vacuum level and the valence level of CuPc overlayers on a V:STO film substrate. The upper panel: vacuum level with reference to that of V:STO, the lower panel: valence level with reference to its Fermi level.

Dielectric Study on Phase Inversion in Microemulsions

Microemulsions are apparently homogeneous mixtures including at least water, oil and surfactant. Some of them show temperature-dependent phase inversion, i.e., the type of emulsions inverts around the temperature at which bicontinuous structure appears, as schematically depicted in Figure 2. The phenomenon that is related to percolation is particularly interesting in view of the dielectric study of heterogeneous systems. In this report, the phase inversion in a ternary mixture of water (10 mM KCl), toluene and Triton X-100 (40: 40: 20 wt %) has been studied by dielectric spectroscopy over a frequency range of 10 Hz to 1 GHz. The transition from the water-in-oil type emulsion to the bicontinuous phase provided maximums for the intensity and the relaxation time of dielectric relaxation, which was accompanied with a steep increase in low-frequency conductivity. The characteristics of the dielectric behavior have been accounted for by interfacial polarization with a percolation model in which spherical water droplets are randomly connected with their nearest neighbors using water bonds.

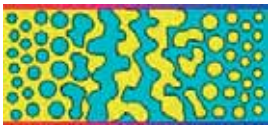

Figure 2. Temperature-dependent phase inversion of microemulsion.

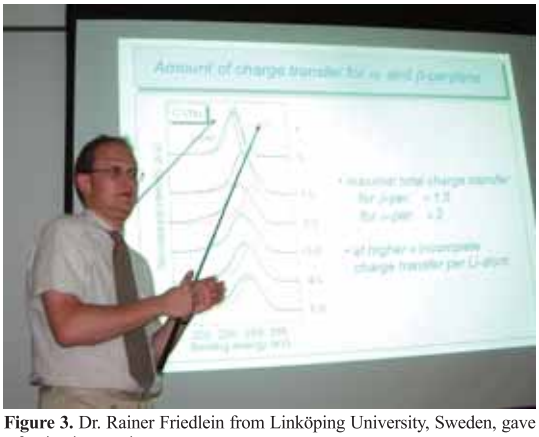

Figure 3. Dr. Rainer Friedlein from Linköping University, Sweden, gave a fascinating seminar.